

CLAIMS:

We claim:

1. A method of initializing a control model for a bioassay process, the method comprising:
preparing a mixture of molecules;
dividing the mixture of molecules into a number of aliquots;
preserving the aliquots of the mixture of molecules;
retrieving at least one aliquot of the preserved mixture;
obtaining data from the at least one aliquot of the preserved mixture using the bioassay process; and
computing a location of a centroid in n-dimensional space based on the data obtained from the at least one aliquot of the preserved mixture, the location of the centroid in n-dimensional space defining the control model.
2. The method of claim 1, wherein said retrieving at least one aliquot includes retrieving two or more aliquots of the mixture of molecules.
3. The method of claim 1, wherein said computing a location of a centroid in n-dimensional space includes:
selecting at least one feature from a plurality of features, the plurality of features being associated with the mixture of molecules;
plotting the at least one feature in n-dimensional space, where n is equal to the number of features selected from the plurality of features; and
computing a location of a centroid based on plots obtained from the plotting.
4. The method of claim 1, wherein the preparing a mixture of molecules includes preparing a mixture of isolated peptides.
5. The method of claim 1, wherein the preparing a mixture of molecules includes preparing a mixture of molecules that are water soluble and have a molecular weight greater than 400.
6. The method of claim 1, wherein the obtaining data using the bioassay process includes obtaining data using an electrospray process.

7. The method of claim 1, wherein the obtaining data using the bioassay process includes obtaining data using a biochip-based process.
8. A method of testing a bioassay process, the method comprising:
retrieving an aliquot of a preserved molecular mixture;
obtaining data from the retrieved molecular mixture using the bioassay process, the data having a plurality of predetermined features; and
determining a distance based on a plotted location of the predetermined features and a predetermined centroid, the centroid being defined in n-dimensional space.
9. The method of claim 8, wherein obtaining data using the bioassay process includes using an electrospray process.
10. The method of claim 8, wherein obtaining data using the bioassay process includes using a biochip.
11. The method of claim 8, wherein retrieving an aliquot of a preserved molecular mixture includes retrieving an aliquot of the same preserved molecular mixture used to create the predetermined control model.
12. The method of claim 8, further comprising:
determining when the obtained data falls within a predetermined distance of a centroid, the centroid defining the predetermined model.
13. The method of claim 12, wherein the determining when the obtained data falls within the predetermined distance including one of: determining that the bioassay process is functioning properly when the obtained data falls within or is equal to the predetermined distance from the centroid, and determining that the bioassay process is not functioning properly when the obtained data falls outside of the predetermined distance from the centroid.
14. The method of claim 8, wherein each of the predetermined features includes a mass-to-charge ratio and a magnitude.

15. A method of testing a bioassay process against a control model, the method comprising:
- preparing a mixture of molecules;
 - dividing the mixture of molecules into a number of aliquots;
 - preserving the aliquots of the mixture of molecules;
 - retrieving at least one aliquot of the preserved mixture;
 - obtaining data from the at least one aliquot of the preserved mixture using the bioassay process;
 - computing a location of a centroid in n-dimensional space based on the data obtained from the at least one aliquot of the preserved mixture, the location of the centroid in n-dimensional space defining the control model;
 - retrieving an aliquot of the preserved molecular mixture at a time following the computing of the control model;
 - obtaining data from the retrieved molecular mixture using the bioassay process, the data having a plurality of predetermined features; and
 - determining a distance based on a plotted location of the predetermined features and a predetermined centroid, the centroid being defined in n-dimensional space.
16. The method of claim 15, wherein obtaining data using the bioassay process includes using an electrospray process.
17. The method of claim 15, wherein obtaining data using the bioassay process includes using a biochip.
18. The method of claim 15, wherein the computing a location of a centroid in n-dimensional space includes:
- selecting at least one feature from a plurality of features, the plurality of features being associated with the mixture of molecules;
 - plotting the at least one feature in n-dimensional space, where n is equal to the number of features selected from the plurality of features; and
 - computing a location of a centroid based on plots obtained from the plotting.

19. The method of claim 15, wherein the at least one feature of the plurality of features are defined by a mass-to-charge ratio and a magnitude.
20. The method of claim 15, wherein retrieving at least one aliquot includes retrieving two or more aliquots of the mixture of molecules.
21. A method, comprising:
retrieving an aliquot of a preserved molecular mixture;
analyzing data from the retrieved molecular mixture using a bioassay process;
comparing a test set of predetermined features of the retrieved molecular mixture with a control set of predetermined features, the control set of predetermined features defining a centroid in n-dimensional space, the test set of predetermined features of the retrieved mixture being the same as the control set of predetermined features; and
determining a degree of error based on a difference between the position of a control centroid, the position of the control centroid being based on the control set of predetermined features and the position of a test centroid, the position of the test centroid being based on the test set of predetermined features of the retrieved molecular mixture.
22. The method of claim 21, wherein said comparing includes comparing a set of mass-to-charge ratios and magnitudes of each of the test set of predetermined features with the mass-to-charge ratios and magnitudes of the control set of predetermined features.
23. The method of claim 21, wherein the analyzing data from the molecular mixture using a bioassay process includes analyzing data from the molecular mixture using an electrospray process.
24. The method of claim 21, wherein the analyzing data from the molecular mixture using a bioassay process includes analyzing data from the molecular mixture using a biochip.